propan-2-yl naphthalen-1-ylacetate 68360-82-7 | DTXSID60286262

68360-82-7	DTXSID60286262

Model Performance

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Weighted KNN model

5-fold CV (5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.81	0.55	0.81	0.54	0.71	0.61	

Model Results

Predicted value: 523 L/kg

Global applicability domain: Inside

Local applicability domain index: 5.39e-01

Confidence level: 5.28e-01

Nearest Neighbors from the Training Set

Image not found

Ethyl 1-naphthaleneacetate

Measured: 302 Predicted: 425

Image not found

Isopropylpropyzamide

Measured: 148 Predicted: 173

Image not found

3,3'-Dichlorobenzidine

Measured: 22400 Predicted: 1680

Image not found

N-Cycloheptyl-N'-phenylurea

Measured: 234 Predicted: 218

Image not found

Carboxin
Measured: 257
Predicted: 210